Convection 1D

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1 Equations

1.1 Mass conservation

$$\frac{\partial c_i}{\partial t} = -\vec{\nabla}.\vec{N}_i + R_i \tag{1}$$

with

$$\vec{N}_i = c_i\vec{v} - \sum_j D_{ij}\vec{\nabla}c_j - w_i c_i \vec{\nabla}U \tag{2}$$

1.2 Poisson's equation

$$\vec{\nabla}^2 U + \frac{F}{\epsilon}\sum_i z_i c_i = 0 \tag{3}$$

1.3 Butler-Volmer kinetics

$$v = k_{ox}\exp\left[\frac{\alpha_{ox}nF}{RT}(V-U)\right]c_{red} - k_{red}\exp\left[-\frac{\alpha_{red}nF}{RT}(V-U)\right]c_{ox} \tag{4}$$

2 Element matrix

2.1 Convection

2.1.1 Fluctuation in node

$$\Delta c_i^m = \sum_e \alpha_e^m \Phi_e$$

2.1.2 Element contribution to fluctuation in node

$$\begin{aligned}
\Phi &= \int_L -\vec{v}.\vec{\nabla}c_i dL \\
&= -\left(\vec{n}^1 c_i^1 + \vec{n}^2 c_i^2\right).\vec{v}_{av} \\
&= -\left(k^1 c_i^1 + k^2 c_i^2\right)
\end{aligned}$$

- One target (e.g. node 1)

$$\alpha^1 = 1$$

$$\alpha^2 = 0$$

$$\left\{ \begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \end{array} \right\} = \left[\begin{array}{cc} -k^1 & -k^2 \\ 0 & 0 \end{array} \right] \left\{ \begin{array}{c} c_i^1 \\ c_i^2 \end{array} \right\} \tag{5}$$

2.1.3 Example: binary electrolyte

- One target (node 1)

$$\left\{ \begin{array}{c} \Delta c_A^1 \\ \Delta c_B^1 \\ \Delta U^1 \\ \Delta c_A^2 \\ \Delta c_B^2 \\ \Delta U^2 \end{array} \right\} = \left[\begin{array}{cccccc} -k^1 & 0 & 0 & -k^2 & 0 & 0 \\ 0 & -k^1 & 0 & 0 & -k^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right] \left\{ \begin{array}{c} c_A^1 \\ c_B^1 \\ U^1 \\ c_A^2 \\ c_B^2 \\ U^2 \end{array} \right\} \tag{6}$$

3 Element jacobian

3.1 Convection

Zero contribution.